



Conference on Ion Chemistry and Mass Spectrometry

Schedule of Presentations

January 17–19, 2020

UCLA Conference Center, Lake Arrowhead, CA

FRIDAY, JANUARY 17

3:30 PM CHECK-IN AND ROOM ASSIGNMENTS

5:00 – 6:30 PM SOCIAL HOUR

POSTER PRESENTERS: Please put your poster up during the welcome social.

6:30 – 8:00 PM DINNER

SESSION I **Presider: Thomas Wyttenbach**

8:00 - 8:25 “Cerium Cation (Ce^+) Reactions with H_2 , D_2 , and HD : CeH^+ Bond Energy and Mechanistic Insights from Guided Ion Beam and Theoretical Studies”, **Maryam Ghassee** and Peter B. Armentrout*, *University of Utah, Salt Lake City, UT*.

8:25 – 8:50 “Entropic Effects in the Collision-Induced Dissociation of Proton-Bound Cytidine Nucleoside Analogue Dimers”, **Yakubu S. Seidu** and Mary T. Rodgers*, *Wayne State University, Detroit, MI*.

8:50 – 9:15 “Amine Walk on a Model Peptoid”, **Yadwinder Singh Mann**, Yuntao Zhang, and Jianhua Ren*, *University of the Pacific, Stockton, CA*.

FRIDAY, JANUARY 17**9:15 – 12:00 PM POSTER SESSION, DRINKS, AND DISCUSSION****POSTER PRESENTATIONS**

1. “Conformations and Protonation Sites of Singly and Doubly Protonated His-His Dipeptide”, **Brandon Stevenson**, Fan Yang, Giel Berden, Jonathan Martens, Jos Oomens, and Peter B. Armentrout*, *University of Utah, Salt Lake City, UT.*
2. “Scrambling of Proline Cis/Trans Isomers During ESI”, **Jacob W. Silzel** and Ryan R Julian*, *University of California, Riverside, CA.*
3. “Revisiting an Old Friend: Using Hybrid QM/MM Methods to Understand the Mechanism of Electron Capture Dissociation of Intact Peptide and Protein Ions”, **Susannah Brown** and William A. Donald*, *University of New South Wales, Sydney, Australia.*
4. “Effect of Metal Ions on Amino Acid Assembly”, **Priyanka Chary** and Michael T. Bowers*, *University of California, Santa Barbara, CA.*
5. CRAFTI and CID: Conformational Studies in Support of Experiment”, **Jacob M. Shaner**, Andrew J. Arslanian, and David V. Dearden*, *Brigham Young University, Provo, UT.*
6. “Thermochemistry for Space Propulsion: Gas-Phase Binding Energies of 1-Alkyl-3-Methylimidazolium Tetrafluoroborate Ionic Liquid Clusters”, Harrison A. Roy, Lucas A. Hamlow, and **Mary T. Rodgers***, *Wayne State University, Detroit, MI.*
7. “Characterization of Potential Thioredoxin-Mimetic Peptides”, **Michael D. Browne** and Jianhua Ren*, *University of the Pacific, Stockton, CA.*
8. “Thermodynamics and Mechanism of Deamidation of H⁺(AsnIle) and H⁺(AsnIleGly)”, **Samantha K. Walker**, Georgia C.Boles, Roland M. Jones III, and Peter B. Armentrout*, *University of Utah, Salt Lake City, UT.*
9. “Utilizing Mass Spectrometry to Elucidate the Structure and Mechanism of the Elusive Protein TagA”, Orlando E. Martinez, **Denise Tran**, Robert T. Clubb, and Joseph A. Loo*, *University of California, Los Angeles, CA.*
10. “Actinide Thermochemistry”, **P. B. Armentrout***, R. M. Cox, A. Kafle, and K. A. Peterson, *University of Utah, Salt Lake City, UT.*

9:15 – 12:00 PM POSTER SESSION, DRINKS, AND DISCUSSION

POSTER PRESENTATIONS (continued)

11. “IMS-MS Study on Selected α -Synuclein Peptides”, **Zhiyuan Zhu**, Anouk M. Rijs, and Michael T. Bowers*, *University of California, Santa Barbara, CA.*

SATURDAY, JANUARY 18

8:00 – 9:00 BREAKFAST

SESSION II Presider: Abraham Badu-Tawiah

9:00 – 9:25 “Alzheimer’s Disease and the Circadian Rhythm: Probing Chemical Changes to Understand Amyloid Induced Toxicity, **Amber L. H. Gray**, Rebecca Prosser, and Thanh Do*, *University of Tennessee, Knoxville, TN.*

9:25 – 9:50 “Neuropeptide: Neuromedin K and Kassinin Reduce Toxicity of A β (25-35) by Different Mechanisms: An Ion Mobility Investigation”, **Xikun Liu**, Michael Tro, and Michael T. Bowers*, *University of California, Santa Barbara, CA.*

9:50 – 10:15 “Mass Spectrometry Determination of Double-Bond Positions in Lipids at the Single-Cell Level”, **Yanlin Zhu**, Wenhua Wang, and Zhibo Yang*, *University of Oklahoma, Norman, OK.*

10:15 – 10:35 BREAK

10:35 – 11:00 “Formation of Oxazolone versus Diketopiperazine: Key Structural Differences and Peptide Sequencing Information”, **Roland M. Jones III**, Georgia C. Boles, and Peter B. Armentrout*, *University of Utah, Salt Lake City, UT.*

11:00 – 11:25 “Elucidating Pathways for the Formation of Internal Fragments Formed from Intact Peptide/Protein Ions”, **Muhammad A. Zenaidee**, Benqiang Wei, Carter Lantz, Taylor Perkins, Rachel R. Loo, and Joseph A. Loo*, *University of California, Los Angeles, CA.*

11:25 – 11:50 “Accelerated Hydrolysis of Lipids by Lipase Enzyme in Charged Droplets”, **Benjamin J. Burris** and Abraham K. Badu-Tawiah*, *Ohio State University, Columbus, OH.*

12:00 – 2:30 LUNCH AND FREE TIME

SATURDAY, JANUARY 18

2:30 – 2:50 **CONFERENCE PHOTO (Please meet in front of Conference center promptly at 2:30 pm so that we can start the afternoon session on time.)**

SESSION III Presider: Thanh Do

3:00– 3:25 “Biomolecular Analysis by SORI-CRAFTI”, **Andrew J. Arslanian**, Caleb Tinsley, Noah Mismash, and David V. Dearden*, *Brigham Young University, Provo, UT*.

3:25 – 3:50 “Improved Multi-Dimensional Detection of Isomers in Crystallin Peptides by TWIM-MS”, **Hoi-Ting Wu** and Ryan R. Julian*, *University of California, Riverside, CA*.

3:50 – 4:15 “UV/Vis Action Spectroscopy of Hydrogen-Deficient Adenine and 9-Methyladenine Cation Radicals in the Gas Phase”, **Shu R. Huang**, Andy Dang, and Frantisek Tureček*, *University of Washington, Seattle, WA*.

4:15 – 4:40 “Absolute Quantitation of Oxidizable Peptides Using Coulometric Mass Spectrometry”, Pengyi Zhao, **Qi Wang**, Richard N. Zare, and Hao Chen*, *New Jersey Institute of Technology, Newark, NJ*.

4:40 – 5:00 BREAK

5:00 – 5:25 “Detergents and Chemical Additives’ Effect on Charge State Distributions During Mass Spectrometry Analysis”, **Wonhyeuk Jung**, Wenzhe Chen, Muhammad Zenaidee, Mark Arbing, Pascal Egea, Rachel R. Loo, and Joseph A. Loo*, *University of California, Los Angeles, CA*.

5:25 – 5:50 “Selective Host-Guest Chemistry, Self-Assembly, and Conformation of m-Xylene Macrocycles Probed by Ion Mobility Mass Spectrometry”, **Benjamin Ayres Link** and Thanh Do*, *University of Tennessee, Knoxville, TN*.

5:50 – 6:15 “Chirality Induced Conformational and Thermochemical Changes in Cysteine Polyalanine Peptides”, **Yuntao Zhang**, Joshua Ho and Jianhua Ren*, *University of the Pacific, Stockton, CA*.

6:30 – 8:00 DINNER

SATURDAY, JANUARY 18

8:00 – 9:30 SATURDAY EVENING LECTURE

Presiding: Mary T. Rodgers

“Atomic Ions to Intact Protein Complexes: 25 Years of IM-MS Development for Ion Structure, Dynamics and Thermodynamics”



David H. Russell
Texas A & M University

**Support for the Saturday evening speaker and celebration generously provided by Bruker
Daltonics, American Elements, and the Waters Corporation.**



9:30 – 12:00

PARTY

SUNDAY, JANUARY 19

8:00 – 9:00 BREAKFAST

SESSION IV Presider: David V. Dearden

9:00 – 9:25 “Uncatalyzed N-Alkylation of Amines in the Gas-Phase Under Ambient Condition: Toward Online Reaction Screening and Product Collection”, **Suji Lee** and Abraham K. Badu-Tawiah*, *Ohio State University, Columbus, OH.*

9:25 – 9:50 “UV-Vis Action Spectroscopy and Energetics of Charge-Tagged Adenosine Radicals”, **Yue Liu**, Andy Dang, and Frantisek Tureček*, *University of Washington, Seattle, WA.*

9:50 – 10:15 “Mass Spectrometry Structural Analysis of Phosphoproteins”, **Carter Lantz**, Muhammad Zenaidee, Denise, Tran, Karl Biggs, Gal Bitan, Rachel R. Loo and Joseph A. Loo*, *University of California, Los Angeles, CA.*

10:15 – 10:35 BREAK

10:35 – 11:00 “Metabolomics Studies of Irinotecan-Resistant Cells under Metformin Treatment”, **Xingxiu Chen** and Zhibo Yang*, *University of Oklahoma, Norman, OK.*

11:00 – 11:25 “Determining Topologies of Alkylammonium Complexes of Curcubit[6]uril Using Multi-CRAFTI Techniques”, **Jamir Shrestha**, Andrew J. Arslanian, Caleb Tinsley, Zixuan Feng, Tina H. M. Farzan, Mariah Pay, and David V. Dearden*, *Brigham Young University, Provo, UT.*

11:25 – 11:50 "Gas-Phase Hydrogen/Deuterium Exchange Behavior of Small Molecules", **Sanjit Uppal**, Abhigya Mookherjee, Rick Harkewicz, Sarah E. Beasley and Miklos Guttman*, *University of Washington, Seattle, WA.*

12:00 CHECK OUT

12:00 – 1:00 LUNCH AND DEPART

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